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DENSITY FUNCTIONAL FOR PAIRING WITH PARTICLE NUMBER CONSERVATION

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In this work, a new functional is introduced to treat pairing correlations in finite many-body systems. Guided by the projected BCS framework, the energy is written as a functional of occupation numbers. It is shown to generalize the BCS approach and to provide an alternative to Variation After Projection framework. Illustrations of the new approach are given for the pairing Hamiltonian for various particle numbers and coupling strengths. In all case, a very good agreement with the exact solution is found.

Keywords: pairing; mesoscopic systems; particle number projection

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1. Introduction

The Nuclear Energy Density Functional (EDF) theory is anticipated to provide a unified framework to describe nuclear structure and reactions. Important efforts are now being made to improve the predicting power of EDF. An important aspect of current EDF is the possibility to break some of the symmetries of the nuclear Many-Body problem in order to grasp specific correlations with rather simple functionals. A typical example is provided by pairing correlations that are approximately treated by relaxing the particle number conservation, like in the BCS or HFB theory. Such theories are expected to be rather effective in the large particle number limit but miss important effects as the particle number and/or coupling decreases. Projection techniques that restore the particle number are expected to significantly improve the description of pairing in that cases¹. Figure 1 illustrates the energy for the "picket fence" pairing Hamiltonian⁸,

$$H = \sum_i \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) - g \sum_{i,j} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j, \quad (1)$$

obtained in the BCS, and projected BCS [PBCS] frameworks when the variation is made before (Variation After Projection [VAP]) or after the variation (Projection After Variation [PAV]). The projection clearly improves the description of correla-

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tion and is almost indistinguishable from the exact result when VAP is performed.

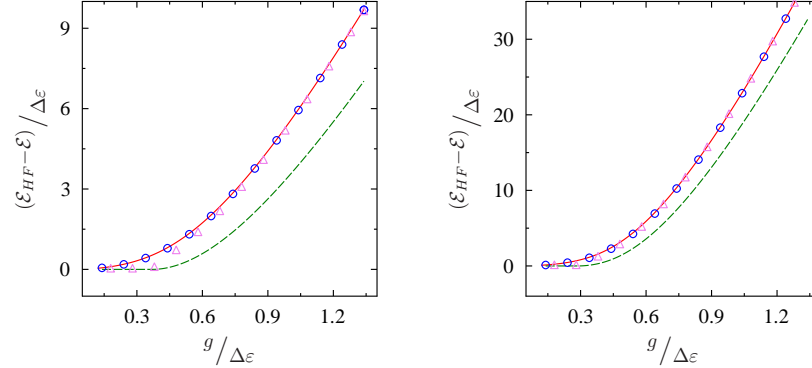


Fig. 1. Difference between the exact total energy and the Hartree-Fock energy (solid line) obtained in the picket fence Hamiltonian with constant level spacing $\Delta\epsilon$ for $A = 8$ and $A = 16$ particles. In both case, the BCS (dashed), PAV (open triangle) and VAP (open circles) results are displayed.

Projection on particle number and/or angular momentum is becoming now a standard tool of nuclear EDF and extensive calculations along the whole nuclear chart is within reach. Recent discussions have however pointed out that projection should be handled with care when combined with functional theory^{2,3}. In particular, specific correction to the so-called self-interaction problem in "GCM like" calculations are necessary^{4,5,6}. In addition, even with proper corrections, projections especially made before the variation⁷ remain very heavy numerically and their use for other problems than nuclear structure, like for instance the dynamics or thermodynamics of nuclear systems, seems difficult. The aim of the present work is to propose a new functional for pairing able to directly grasp correlations generally incorporated through projection by specific dependence on the the natural occupation numbers n_i and orbitals $\{\varphi_i\}$, i.e. $\rho = \sum_i |\varphi_i\rangle n_i \langle \varphi_i|$ where ρ denotes the exact one body density matrix.

2. Density Matrix Functional for pairing

Our starting point is the projected BCS state given by:

$$|N\rangle \equiv \frac{1}{\sqrt{N!}} \left(\sum_i x_i a_i^\dagger a_i^\dagger \right)^N |-\rangle, \quad (2)$$

where $\{a_i^\dagger, a_i^\dagger\}$ denotes pairs of time-reversed states. It could easily be shown that this state can be obtained by projection of the BCS state, $|\text{BCS}\rangle = \prod (1 +$

$x_i a_i^\dagger a_i^\dagger |0\rangle|-\rangle$, onto good particle number $A = 2N$. Note that here N denotes the number of pairs. The PBCS energy for the Hamiltonian (1) reads

$$\frac{\langle N|H|N\rangle}{\langle N|N\rangle} \equiv \mathcal{E}(n_i, C_{ij}) = 2 \sum_i \varepsilon_i n_i - g \sum_{ij} C_{ij}, \quad (3)$$

where n_i and C_{ij} are the occupation probabilities and correlation matrix elements defined through

$$n_i = \frac{\langle N|a_i^\dagger a_i|N\rangle}{\langle N|N\rangle}, \quad C_{ij} = \frac{\langle N|b_i^\dagger b_j|N\rangle}{\langle N|N\rangle}. \quad (4)$$

According to the definition (2), n_i and C_{ij} and therefore $\mathcal{E}(n_i, C_{ij})$ can eventually be written as an explicit functional of the $\{x_i\}$ parameters, which turns out to be too complicated for a direct use as variational parameters. After tedious manipulation, it has been shown in ref. ⁹, that these parameters can approximately be written as a functional of the $\{n_i\}$ through:

$$|x_i|^2 \simeq \left(\frac{n_i}{1 - n_i} \right) (a_0 - a_1 n_i) \quad (5)$$

with

$$a_1 = \frac{1}{N} (1 + s_2 + s_2^2 + \dots + s_2^{N-1}) = \frac{1}{N} \frac{1 - s_2^N}{1 - s_2} \quad (6)$$

and

$$a_0 = 1 + \frac{(s_2 - s_3)}{N} (1 + 2s_2 + \dots + (N-1)s_2^{N-2}) = 1 + (s_2 - s_3) \frac{\partial a_1}{\partial s_2}, \quad (7)$$

and $s_p = 1/N \sum n_i^p$. With these expressions, we can now write the correlation as a functional of single-particle occupancies:

$$C_{ij} = \sqrt{n_i(1 - n_i)n_j(1 - n_j)} \times \frac{\sqrt{(a_0 - a_1 n_i)(a_0 - a_1 n_j)}}{\{a_0 - a_1(n_i + n_j - n_i n_j)\}}. \quad (8)$$

The present functional, based on the PBCS trial state, corresponds to a generalization of the BCS ansatz that approximately account for particle number conservation. The BCS limit is obtained for $a_0 = 1$ and $a_1 = 0$ leading to the well know expression $C_{ij} = \sqrt{n_i(1 - n_i)n_j(1 - n_j)}$. It is worth to mention that a completely different expression is obtained in the weak coupling limit (Hartree-Fock limit) for which $s_2 = s_3 = 1$ and $C_{ij} \rightarrow \sqrt{n_i n_j}$.

Illustrations of the new functional accuracy are given in figure 2 where the energy is obtained by a direct minimization of (3) using expression (8). A very good agreement is obtained for any particle number and coupling strength.

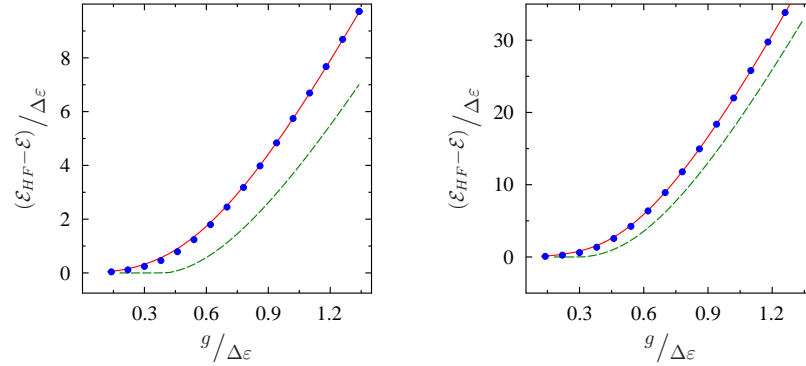
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Fig. 2. Same quantity as in Figure 1 displayed as a function of the coupling strength for the exact (solid line), BCS (dashed line) and the new functional (filled circles) case.

3. Summary

Following the Density Matrix Functional Theory spirit¹⁰, the possibility to use functionals of natural orbitals and occupancies has been recently introduced in nuclear physics^{11,12}. In the present work, a new functional for pairing is introduced that corrects the BCS theory for particle number conservation effects. The present framework provides an alternative way to perform VAP calculations and is expected (i) to greatly simplify such calculation compared to direct use of projection operator, (ii) to directly give access to physical quantities like natural occupancies, (iii) to be particularly suitable for EDF based theories.

References

1. P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer Verlag, 1980).
2. M. Anguiano, J. L. Egido, and L.M. Robledo, *Nucl. Phys. A* **696**, 467 (2001).
3. J. Dobaczewski, M. V. Stoitsov, W. Nazarewicz, and P. G. Reinhard, *Phys. Rev. C* **76**, 054315 (2007).
4. D. Lacroix, T. Duguet, and M. Bender, *Phys. Rev. C* **79**, 044318 (2009).
5. M. Bender, T. Duguet, and D. Lacroix, *Phys. Rev. C* **79**, 044319 (2009).
6. T. Duguet, M. Bender, K. Bennaceur, D. Lacroix, and T. Lesinski, *Phys. Rev. C* **79**, 044320 (2009).
7. J. A. Sheikh and P. Ring, *Nucl. Phys. A* **665**, 71 (2000).
8. R. W. Richardson and N. Sherman, *Nucl. Phys.* **52**, 221 (1964). R. W. Richardson, *Phys. Rev.* **141**, 949 (1966). R. W. Richardson, *J. Math. Phys.* **9**, 1327 (1968).
9. D. Lacroix and G. Hupin, arXiv:1003.2860.
10. T. L. Gilbert, *Phys. Rev. B* **12**, 2111 (1975).
11. T. Papenbrock and A. Bhattacharyya, *Phys. Rev. C* **75**, 014304 (2007). M. G. Bertolli and T. Papenbrock, *Phys. Rev. C* **78**, 064310 (2008).
12. D. Lacroix, *Phys. Rev. C* **79**, 014301 (2009).

